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Effects of Pressure, Temperature and Dilution on Fuels/Air Mixture Laminar Flame Burning Velocity

Sebastian Brusca[a], Rosario Lanzafame[b], Adriana Marino Cugno Garrano[b]*, Michele Messina[b]

[a]*University of Messina, C.da Di Dio, 98166 Messina*
[b]*University of Catania, V.le A. Doria 6, 95125 Catania*

Abstract

Fuel laminar burning velocity is an important parameter in internal combustion engine modeling and combustion analysis.
The present paper deals with the development of a mathematical correlation able to provide laminar burning velocity for fuels/air mixture at different thermodynamic conditions. Therefore, a mathematical investigation of laminar burning velocity for most significant and used fuels was carried out.
Fifth order logarithmic polynomial functions were implemented to predict the propagating laminar burning velocity of combusting fuels as a function of equivalent ratio at different conditions of temperature and pressure.
On the basis of results obtained, the mathematical model proposed in this paper showed a higher precision in experimental data fitting and the possibility to interpolate and use a single mathematical function for a wider operation field.

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Keywords: matematical modelling; combustion; laminar burning velocity; equivalence ratio; fuels

1. Introduction

The laminar burning velocity is an important parameter that can be used for both practical applications and theoretical model of internal combustion engines and burners. Most of combustion system mathematical models use this parameter to determine turbulent flame front velocity [1]. Both Internal

* Corresponding author. Tel.: +39 095 7382455; fax: +39 095 337994.
E-mail address: amarin@dii.unict.it.

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combustion Engine (ICE) and Combustion Turbine (CT) mathematical modeling needs to take into account laminar flame velocity in the equations. That is much more important in combustion studies of not conventional fuels [2] and synthesis gas [3, 4]. Several authors measured laminar burning velocity for a wide variety of fuels as a function of equivalence ratio and highlighted its strong temperature and pressure dependence [5 – 10].

The most common relation used to fit flame burning velocity data for hydrogen, methane, propane, iso-octane, methanol and gasoline, at different pressure and temperature of unburned mixture, is a power law of temperature and pressure where exponents are a function of equivalence ratio. This power law also depends on the laminar velocity at reference conditions (S_{L0}). Iijima et al. [5] proposed an expression for temperature and pressure exponents that linearly depend on the equivalence ratio, used by most of authors [5 – 10]. Metghalchi et al. [6 – 7] used a second-order polynomial function of fuel ratio for laminar flame velocity at the reference conditions for methanol, isooctane, indolene and propane, while Galmiche et.al used a forth-order polynomial function for iso-octane [8]. Verea et al. recently extended the linear power exponent of pressure to contain quadratic term of equivalence ratio. During their calculation for n-butanol, iso-octane, Liu K. et al. [9] found that it is difficult to compromise such range of equivalence ratio of interest unless the power exponent of pressure is extended to include the cubic term. Ravi et al. [10] assumed the laminar velocity at reference conditions and the two exponents to be different order polynomial functions of equivalence ratio for hydrogen-oxygen mixture. To cover whole range of equivalence ratio data, Ravi et al. used different polynomial functions calculating the corresponding coefficients.

In the present work the authors proposed a mathematical method to describe the flame burning velocity as a function of equivalence ratio, pressure and temperature. The method is based on fifth order logarithmic polynomial functions (VoLP) to define the laminar velocity at the reference conditions and for both power exponents of pressure and temperature. VoLP function application presents several mathematical advantages as widely described in [11 - 14]. Laminar burning velocities of several fuels were determined on the basis of experimental data in order to verify method efficacy and precision. Considering the registered errors it can be stated that the mathematical model accurately describes the laminar burning velocity behavior as a function of equivalence ratio, at different pressure and temperature condition in all combustion engineering range.

This method allows predicting laminar burning velocity of combusting air/fuel mixtures in several engineering applications. In particular, in ICE modeling it is necessary to know laminar burning velocity as a function of local equivalence ratio, as well as pressure and temperature in order to calculate turbulent flame speed. The present work represents a first step in a wider research to model combustion in ICE running on non-conventional fuels.

Nomenclature

S_L	laminar burning velocity [cm/s]
α	power exponent of temperature
β	power exponent of pressure
ϕ	equivalence ratio
T	temperature [K]
p	pressure [atm]
X	coefficient matrix

Y	result data vector
A	VoLP coefficient vector at reference conditions
B	VoLP coefficient vector at arbitrary conditions
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0	reference conditions
Tp	generic pressure and temperature conditions

2. Fifth order logarithmic polynomial mathematical model

The laminar velocity simultaneous dependence in temperature and pressure was taken into account by authors employing the common function described by a power law expression as in equation (1).

$$S_L = S_{L0}\left(\frac{T}{T_0}\right)^{\alpha}\left(\frac{p}{p_0}\right)^{\beta} \tag{1}$$

where SL is the laminar burning velocity at arbitrary conditions of temperature (T) and pressure (p), T0 and p0 are the reference temperature and pressure, SL0 is the laminar burning velocity at reference conditions, α and β are respectively the power exponent of temperature and pressure. In this paper fifth order logarithmic polynomial functions are proposed to define the laminar velocity SL0 and the exponent α and β as a function of equivalence ratio ϕ (see equation (2)).

$$S_L(\phi) = \left(\sum_{i=0}^{5} a_i\,(\ln\phi)^i\right)\left(\frac{T}{T_0}\right)^{\left(\sum_{i=0}^{5} b_i(\ln\phi)^i\right)}\left(\frac{p}{p_0}\right)^{\left(\sum_{i=0}^{5} c_i(\ln\phi)^i\right)} \tag{2}$$

Coefficients “ai”, “bi“ and “ci“ are determined for a given fuel with the least square method by fitting experimental data. The calculation procedure of all coefficients for each fuel consists in three main steps.

The coefficients “ai“ are firstly obtained starting from the experimental data of the laminar burning velocity at reference conditions and solving the over-determined matrix system (3).

$$Y_0 = X_0\,A \tag{3}$$

where

$$Y_0 = \begin{bmatrix} S_{L0}(\phi_1) \\ S_{L0}(\phi_2) \\ . \\ . \\ . \\ S_{L0}(\phi_n) \end{bmatrix} \tag{4}$$

column vector of experimental data $S_{L0}(\phi_j)$ at reference temperature and pressure (T0, p0) (j=1,2,…n) with n>5

$$X_0 = \begin{bmatrix} 1 & ln\phi_1 & (ln\phi_1)^2 & (ln\phi_1)^3 & (ln\phi_1)^4 & (ln\phi_1)^5 \\ 1 & ln\phi_2 & (ln\phi_2)^2 & (ln\phi_1)^3 & (ln\phi_1)^4 & (ln\phi_1)^5 \\ & & & \vdots & & \\ 1 & ln\phi_n & (ln\phi_n)^2 & (ln\phi_n)^3 & (ln\phi_n)^4 & (ln\phi_n)^5 \end{bmatrix} \quad (5)$$

with ϕ_j data values of equivalence ratio (j=1,2,…n)

A is the column vector of unknown coefficients ai of fifth order logarithmic polynomial relative to laminar burning velocity at reference conditions. It is determined by solving the matrix system (6).

$$A = \left({X_0}^T X_0\right)' {X_0}^T Y_0 \quad (6)$$

where X_0T is the matrix transpose of X_0 and (X_0TX_0)' is the matrix inverse of (X_0TX_0).

Secondly, the temperature exponent coefficients bi and the pressure exponent coefficients ci are determined by the matrix system (7).

$$B = \left({X_{Tp}}^T X_{Tp}\right)' {X_{Tp}}^T Y_{Tp} \quad (7)$$

where B is the column vector of unknown coefficients bi and ci of fifth order logarithmic polynomial relative to temperature and pressure exponents.

$$Y_{Tp} = \begin{bmatrix} ln\left(\frac{S_{LTp}(\phi_1)}{S_{L0}(\phi_1)}\right) \\ ln\left(\frac{S_{LTp}(\phi_2)}{S_{L0}(\phi_2)}\right) \\ \vdots \\ ln\left(\frac{S_{LTp}(\phi_m)}{S_{L0}(\phi_m)}\right) \end{bmatrix} \quad (8)$$

$$X_{Tp} = \left[X_T\, X_p\right] \quad (9)$$

where:

$$X_T = \begin{bmatrix} ln\left(\frac{T}{T_0}\right) & ln\left(\frac{T}{T_0}\right)\cdot ln\phi_1 & ln\left(\frac{T}{T_0}\right)\cdot (ln\phi_1)^2 \dots\dots\dots\dots ln\left(\frac{T}{T_0}\right)\cdot (ln\phi_1)^5 \\ & & \vdots \\ ln\left(\frac{T}{T_0}\right) & ln\left(\frac{T}{T_0}\right)\cdot ln\phi_m & ln\left(\frac{T}{T_0}\right)\cdot (ln\phi_m)^2 \dots\dots\dots\dots ln\left(\frac{T}{T_0}\right)\cdot (ln\phi_m)^5 \end{bmatrix} \quad (10)$$

$$X_p = \begin{bmatrix} ln\left(\frac{p}{p_0}\right) & ln\left(\frac{p}{p_0}\right)\cdot ln\phi_1 & ln\left(\frac{p}{p_0}\right)\cdot (ln\phi_1)^2 \dots\dots\dots\dots ln\left(\frac{p}{p_0}\right)\cdot (ln\phi_1)^5 \\ & & \vdots \\ ln\left(\frac{p}{p_0}\right) & ln\left(\frac{p}{p_0}\right)\cdot ln\phi_m & ln\left(\frac{p}{p_0}\right)\cdot (ln\phi_m)^2 \dots\dots\dots\dots ln\left(\frac{p}{p_0}\right)\cdot (ln\phi_m)^5 \end{bmatrix} \quad (11)$$

with T and p arbitrary temperatures and pressures, $S_{LTp}(\phi_k)$ experimental data of laminar velocity at the arbitrary temperatures and pressures (T, p), ϕ_k data values of equivalence ratio (k=1,2,….m), $S_{L0}(\phi_k)$ laminar velocity values at reference conditions (T0, p0) calculated using equivalence ratio data ϕ_k and coefficients "ai" in equation (3).

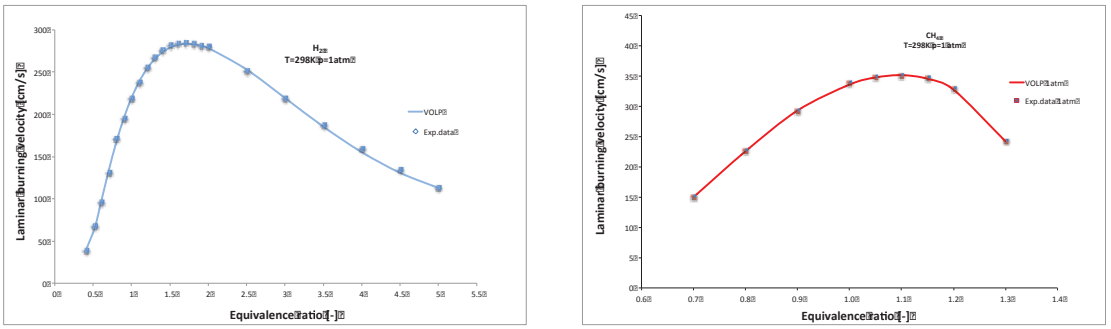
3. Results and discussion

Experimental data from literature [15 – 17] for different fuels were used to determine all coefficients and validate the mathematical model proposed by authors. Validation model results are shown, as an example, for hydrogen, methane and iso-octane.

The constant coefficients "ai" were determined by means of laminar burning velocity data set of hydrogen and methane at reference conditions T0 = 298 K and p0 = 1 atm [15, 16]. The comparison between experimental data and the correlation curves is shown in Fig. 1 with an average error less than 1%.

In the following, hydrogen, methane and iso-octane data were used to calculate coefficients. Therefore, parameters "bi" were calculated for hydrogen using experimental data set at reference pressure and variable temperature of 303 K, 373 K, and 443 K. Moreover, parameters "ci" were calculated for methane at reference temperature and variable pressures of 5 and 10 atm [16, 17].

In the graphs in Fig. 2, hydrogen laminar burning velocity is reported as a function of equivalence ratio at mentioned temperatures (Fig. 2a) while methane laminar burning velocity at above mentioned pressures (Fig. 2b). In the same figures experimental data and interpolation curves are shown. It is well evident that interpolation curves match experimental data very well (average relative error of about 5.71 % and 1.35 % for Fig.2a and Fig. 2b, respectively).



(a) (b)

Fig. 1. Experimental and calculated laminar burning velocity as a function of equivalence ratio at reference conditions (hydrogen (a), methane (b))

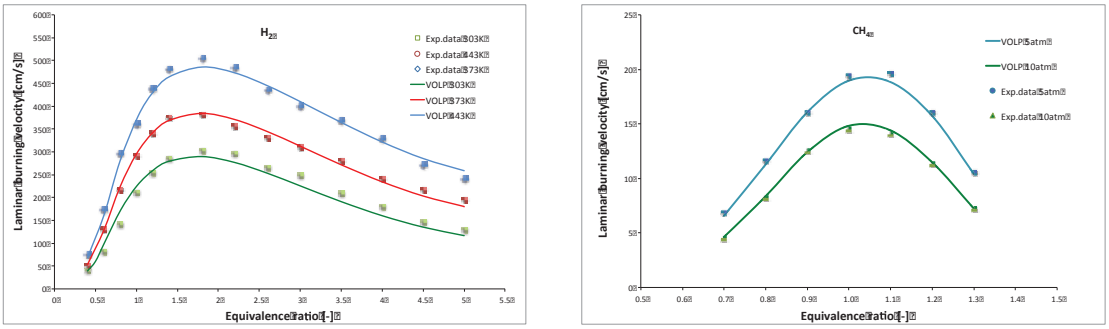


Fig. 2. Comparison between experimental and calculated laminar burning velocity as a function of equivalence ratio at different temperatures for hydrogen (a) and at different pressures for methane (b)

To test extrapolation capabilities of the proposed mathematical model iso-octane results were used. The efficacy validation is shown extrapolating several curves at different pressures and temperatures (see Fig. 3). The extrapolations were carried out using the coefficients “ai”, “bi”, “ci” determined using experimental data set of iso-octane at reference conditions T0 = 323 K and p0 = 1 bar, at reference pressure and variable temperature of 373 K, 423 K, and 473 K, as well as at reference temperature and variable pressures of 2, 3, 5, and 10 bar, respectively [8]. In particular, Fig. 3a, 3b, 3c and 3d show laminar burning velocity as a function of equivalence ratio at different reactant temperatures (323 K, 373 K, 423 K and 473 K) and at different reactant pressures (2 bar, 3 bar, 5 bar and 10 bar). In the same figures experimental data and interpolation curves are reported.

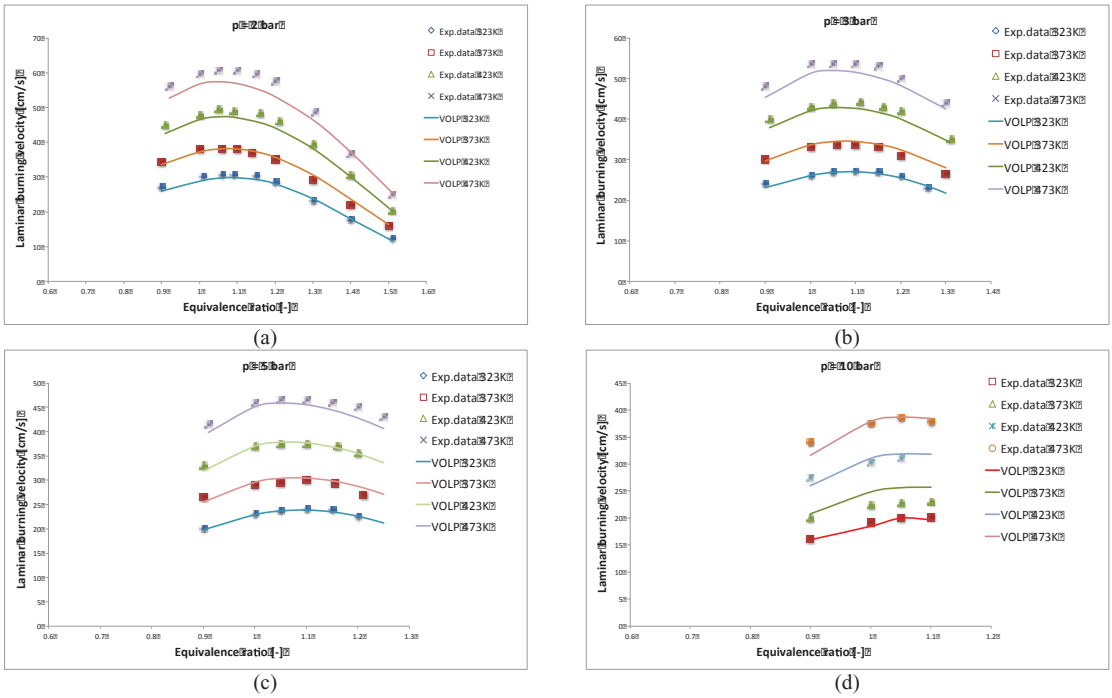


Fig. 3. Experimental and calculated laminar burning velocity as a function of equivalence ratio at different pressures and

temperatures

Result analysis leads to the consideration that laminar burning velocity increases with equivalence ratio up to a maximum and then decreases while equivalence ratio still increases. This behavior is well evident for all analyzed fuels at different pressures and temperatures. Moreover, increasing reactant pressure (Fig. 2b and Fig. 3) a reduction in laminar burning velocity is observed at all equivalence ratios. Temperature effects on laminar burning velocity are well evident in Fig. 3. A higher reactant temperature has the effect to speed up the combustion reaction increasing the laminar burning velocity. This behavior is observed for all studied reactant pressures, as well as at all equivalence ratios. As far as the extrapolation capabilities it is concerned, it is possible to observe that extrapolating the curves for each pressure the average error increases with temperature, while increasing the pressure the extrapolation errors are almost constant for each temperature.

In conclusion, on the basis of the presented results, it is possible to state that the proposed mathematical model is able to predict laminar burning velocity as a function of equivalence ratio, pressure and temperature with a good agreement with experimental data. Thus, the mathematical model is validated.

4. Conclusions

The present paper deals with the study of laminar burning velocity of fuels as a function of equivalence ratio, as well as reactant pressure and temperature. Therefore, a mathematical model to interpolate and extrapolate experimental data was proposed and tested. In the comparison between experimental data and simulated results, an average relative error of about or less than 2% was registered at reference conditions. Thus, on the basis of the errors the proposed model is validated.

In order to verify extrapolation capabilities, several tests were carried out at different pressure and temperature. Results analysis highlighted that the proposed mathematical model is able to extrapolate data for reactant pressure and temperature with low errors (maximum average error registered less than 4%).

Coefficients determination for several fuels was carried out. For each studied fuel, reference, pressure and temperature coefficients were determined starting from experimental data.

On the basis of the presented results it is possible to state that the proposed mathematical model is able to predict laminar burning velocity of fuel/air mixture in all interest equivalence ratio, pressure and temperature ranges with very low errors. Moreover, it is able to do that just using a single function.

5. Copyright

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Biography

Adriana Marino Cugno Garrano is a researcher in energy systems and environment at the University of Catania. She is involved in research on the topics of Internal Combustion Engines and Gas Turbine, combustion, alternative fuels, as well as advanced materials. The research includes the theoretical, algorithmic and applied aspects.